2-hydroxy-3-methyl-2-(propan-2-yl)butanoic acid
5438-17-5 | DTXSID50280375

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.86

Global applicability domain: Inside

Local applicability domain index: 4.41e-01

Confidence level: 8.03e-01

Nearest Neighbors from the Training Set

Image not found
Phenylphosphinic acid
Measured: 6.03
Predicted: 4.42

Image not found
Benzoic acid, 4-(methylamino)-
Measured: 2.40
Predicted: 4.00

Image not found
2,2-Dimethylpropanoic acid
Measured: 2.29
Predicted: 2.74

Image not found
3-Nitrobenzoic acid
Measured: 7.08
Predicted: 3.63

Image not found
3-Hydroxy-2-naphthoic acid
Measured: 3.98
Predicted: 3.94